Techniques for Quality Assurance of Models in a Multi-Run Simulation Environment

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Abstract

In this paper the multi-run simulation experiment environment SimEnv and its application on quality assurance matters of models is described. SimEnv has been designed to provide key working techniques for experimenting with complex models. This includes a wide range of simulation and model output evaluation methods in combination with appropriate visualization techniques. The SimEnv framework allows easily to carry out multi-run model simulation experiments for standardized, pre-formed experiment types. Coupling of models to the environment is supported by a simple interface, requiring only minimal model source code modifications.
Uncertainty and sensitivity analyses are enabled in SimEnv by combining experiments from the set of pre-defined experiment types with interactive post-processing, applying sequences of related operators to both model output and reference data.
Usage of SimEnv as an experimental framework for models in global change research demonstrates the applicability of the approach to multi-input / multi-output problems with large amount of spatio-temporal model output and emphasizes the importance of graphical result presentation and evaluation by appropriate visualization techniques.

Model Application in Global Change Research

Model design, simulation and evaluation are cornerstones in climate impact and global change research. In the past, chains of stand-alone model simulations have been performed to derive from an input scenario (e.g., of greenhouse gas emission over time) of one model from this chain model outputs (e.g., climate change over time) that are used as inputs to the succeeding model. Finally, the complete system can be studied and investigated this way. Nowadays, one of the challenges in global change research is development of integrated models, which is mainly brought about by additional knowledge gained through feedbacks between the studied sub-systems on one hand and through increasing computing power on the other hand.

Such complex simulation models often base on legacy source code applications written in a programming language rather than in a model design language, and they produce large amounts of model output that has to be handled in the course of model validation and/or corroboration. Application of quality assurance techniques to this kind of models is hampered by the elucidated aspects since source code is not so well-known or partially unavailable and intensive code manipulations are normally out of the scope. Additionally, computational costs for models in global change are often very high, demanding structured experimentation approaches.

SimEnv Approach

SimEnv (Flechsig *et al.*, 2003) has been developed to provide a toolbox-oriented simulation environment that enables the modeller and/or model user to deal with model-related quality assurance matters and scenario analyses for the model classes described above. Both foci require flexible experiment design and model output evaluation for model inspection, validation / corroboration, uncertainty and sensitivity analyses as well as for control design without necessarily to change a complex model in general.

The SimEnv approach to couple models to the simulation environment is based on minimal source code adaptations,

- to map targets (input factors), the modeller wants to experiment with and their numerical adjustments from the simulation environment to the model and
- to store (n-dimensional) state variables (outputs) in self-describing Network Common Data Form NetCDF format (NetCDF, 2003) for later post-processing.

The model coupling interface is available for models written in C, Fortran, Python, GAMS and at the command shell level and supports all numerical data types. The model itself can be distributed across platforms as a set of interacting sub-models.

SimEnv aims at simulation studies including well-tailored evaluation approaches with a model in a co-ordinated manner by performing run ensembles instead of single simulation runs. Co-ordination is achieved by pre-defined experiment types representing multi-run simulations. According to the strategy of a selected experiment type the experiment targets (a subset of model parameters, drivers, initial and/or boundary values) are re-adjusted numerically before each single simulation run of the run ensemble is performed. Experiment types implemented so far are

- Behavioural analysis:
  Inspection of the model's behaviour in a multi-dimensional target space with deterministic numerical adjustments and a flexible screening strategy
- Sensitivity analysis:
  Study of the model's behaviour in a local neighbourhood of the control scenario (point of target default values in the target space)
- Monte-Carlo analysis:
  Perturbation of correlation-free targets according to pre-defined distributions using different target sampling methods
- Simulation based optimization:
  Application of gradient-free methods to optimize a cost function

After plugging the model into SimEnv by the implementation of function calls in the source code to transmit the target values and to gather the desired outputs under consideration the modeller has to select a standardized experiment type and has to specify the targets involved in the experiment and the target parameters during experiment preparation. For example, for a Monte-Carlo analysis the distributions together with their distribution parameters to be applied to the targets as well as the number of runs and the target sampling method for the complete experiment have to be declared.

The single simulation runs of the entire run ensemble can be performed either in sequential mode or as a parallel experiment using generic Message Passing Interface MPI to distribute single runs across a network of interacting compute resources.

Uncertainty and Sensitivity Analyses

Exploration of the model output variables' set from the run ensemble of a selected experiment type during result post-processing and evaluation is the key methodical approach for uncertainty and sensitivity analyses in SimEnv. Derived from the general experiment layout, SimEnv experiment types are associated with uncertainty and sensitivity analyses techniques in the following way:

- Behavioural analysis:
  Can be used for uncertainty analysis, factorial screening, general one-factor-at-a-time approach, (fractional) factorial experiments and response surface methodology. All methods can benefit from the flexible screening strategy of multi-dimensional target spaces in SimEnv.
- Sensitivity analysis:
  Can be used for local first order sensitivity analysis by finite difference approximations of derivatives
- Monte-Carlo analysis:
  Can be used for uncertainty analysis and global sensitivity analysis

Interactive post-processing is applied to compute output functions from the model's output by state space transformation operators and to derive uncertainty and sensitivity measures from these output functions by experiment type-specific operators. For this purpose, the SimEnv post-processor enables application of operator sequences to both model output and reference data. Currently, about 100

operators are built in the post-processor. There is an interface to easily declare user-defined operators and plug them into the environment.

State space transformation operators cover among others elemental, analytical, statistical (state variable aggregations over all dimensions), and selective (state variable clipping and partial aggregations for selected dimensions) techniques. Main focus is on a reduction and aggregation in the output model state space to cope with its high dimensionality and extent.

Normally, sensitivity and uncertainty operators are applied to output functions generated by state space transformation operators. For local sensitivity analysis a set of sensitivity measures (linear, squared, absolute, relative, symmetric) are at disposal. Global sensitivity analysis enables among others computation of extremes, moments, quantiles, heuristic probability density functions from targets (input factors) and output functions as well as linear regression analysis and correlation and covariance measures between targets, output functions and both.

Potential demand for specific operators can be fulfilled in two ways: by wrapping appropriate techniques into an operator and using it as a plug-in for the post-processor or by exporting post-processor output in NetCDF format and forwarding it to special-purpose tools.

Analysis and evaluation of post-processed data selected and derived from large amount of relevant model output benefits from visualization techniques. Based on metadata information of the post-processed experiment type, the applied operator chain, and the dimensionalities of the post-processor output pre-formed visualization modules are evaluated by a suitability coefficient how they can map the data in an appropriate manner.

The visualization modules offer a high degree of user support and interactivity to cope with multi-dimensional data structures. They cover among others standard techniques such as scatter and parallel coordinate (cobweb) plots (for abstract data visualization), and isolines, isosurfaces, direct volume rendering and a 3D difference visualization technique (for spatial and temporal data visualization). Furthermore, approaches to navigate intuitively through large multi-dimensional data sets have been applied, including details on demand, interactive filtering and animation. Using the visualization platform OpenDX (OpenDX, 2003) from IBM extended OpenDX techniques have been designed and implemented, suited in the context of analysis and evaluation of simulated multi-run output functions.

Applications

SimEnv has been applied among others to study uncertainty in an earth system model of intermediate complexity (Petoukhov *et al.*, 2000) and to determine its climate sensitivity (Schneider von Deimling & Held, 2003). The paper will show from an ongoing study sensitivity results for a regional meteorological model (Doms & Schättler, 1997) in climate mode (Kücken & Hauffe, 2002) where physical and numerical parameters subsets in their relation to diagnostic and prognostic model output variables have been under investigation.

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